# Jaguar 7.6

## Quick Start Guide

Schrödinger Press

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# Contents

# Document Conventions

In addition to the use of italics for names of documents, the font conventions that are used in this document are summarized in the table below.

| Font | Example | Use |
|---|---|---|
| Sans serif | Project Table | Names of GUI features, such as panels, menus, menu items, buttons, and labels |
| Monospace | `$SCHRODINGER/maestro` | File names, directory names, commands, environment variables, and screen output |
| Italic | *filename* | Text that the user must replace with a value |
| Sans serif uppercase | CTRL+H | Keyboard keys |

Links to other locations in the current document or to other PDF documents are colored like this: Document Conventions.

In descriptions of command syntax, the following UNIX conventions are used: braces `{ }` enclose a choice of required items, square brackets `[ ]` enclose optional items, and the bar symbol | separates items in a list from which one item must be chosen. Lines of command syntax that wrap should be interpreted as a single command.

File name, path, and environment variable syntax is generally given with the UNIX conventions. To obtain the Windows conventions, replace the forward slash / with the backslash \ in path or directory names, and replace the $ at the beginning of an environment variable with a % at each end. For example, `$SCHRODINGER/maestro` becomes `%SCHRODINGER%\maestro`.

In this document, to *type* text means to type the required text in the specified location, and to *enter* text means to type the required text, then press the ENTER key.

References to literature sources are given in square brackets, like this: [10].

# Getting Started

This manual contains exercises designed to help you learn the basic tasks you will need to prepare and initiate Jaguar calculations from Maestro. For more information about Jaguar features, see the *Jaguar User Manual*.

This chapter contains instructions for setting up the tutorial.

Chapter 2 contains exercises on building new molecular structures, which are used in the calculations in the next chapter.

Chapter 3 provides a set of exercises that show you how to run various Jaguar calculations: single-point energies with both DFT and LMP2 theory, geometry optimizations, transition state searches, intrinsic reaction coordinate calculations, frequency calculations, orbital plotting, and p$K_a$ prediction.

Help for each of the Jaguar tasks is available in the Maestro online help.

To do the exercises, you must have access to an installed version of Maestro 9.0 and Jaguar 7.6. For installation instructions, see the *Installation Guide*. The directory in which the software is installed will be referred to as the installation directory.

The preparations that must be made for the exercises are to create a working directory to keep all your input and output files, start Maestro, ensure that this directory is Maestro's current working directory, and create a project. These tasks are described in the following sections.

## 1.1 Creating a Working Directory

The first task to be done in preparation for the tutorial is to create a working directory to keep all your input and output files.

**UNIX:**

1. Change to a directory in which you have write permission.

   `cd` *mydir*

2. Create a directory by entering the command:

   `mkdir` *directory-name*

**Windows:**

1. Open the folder in which you want to create the folder that serves as your working directory.

   The default working directory used by Maestro is your user profile, which is usually set to `C:\Documents and Settings\`*username* on Windows XP and 2000, and to `C:\Users\`*username* on Vista. To open this folder, do the following:

   a. Choose Run from the Start menu.

   b. Enter `%USERPROFILE%` in the Open text box and click OK.

2. Click Make a new folder under File and Folder Tasks.

   You can also choose Folder from the New submenu of the File menu.

3. Enter a name for the folder.

   If you want to create a folder inside this folder, repeat this procedure.

## 1.2 Starting Maestro

Once you have created the working directory you can start Maestro.

**UNIX:**

1. Set the `SCHRODINGER` environment variable to the installation directory:

   **csh/tcsh:** `setenv SCHRODINGER` *installation_path*
   **bash/ksh:** `export SCHRODINGER=`*installation_path*

   This environment variable is also required to run Jaguar jobs.

2. Change to the desired working directory.

   `cd` *directory-name*

3. Enter the command:

   ```
   $SCHRODINGER/maestro &
   ```

   The Maestro main window is displayed, and the working directory is Maestro's current working directory.

**Windows:**

- Double-click the Maestro icon on the desktop.

  You can also use the Start menu. Maestro is in the Schrödinger submenu.

## 1.3 Setting the Maestro Working Directory

If you are running Maestro under Windows, or if you are using an existing Maestro session under UNIX, you must change to the working directory that you created for the tutorial in Section 1.1.

1. Choose Change Directory from the Maestro menu.
2. Navigate to the appropriate directory and click OK.

## 1.4 Creating a Maestro Project

When you start Maestro, a scratch project is created. This project must be named in order to keep it for later use. You should therefore create a named Maestro project to save the structures that you build, in case you want to complete the exercises at a later time. For more information on Maestro projects, see Chapter 8 of the *Maestro User Manual*.

1. Choose Save As from the Project menu.

   The Save Project dialog box is displayed. The Look in option menu should contain the current Maestro working directory.

2. In the File name text box, type `JaguarTutorial`.
3. Click Save.

This procedure creates a project named `JaguarTutorial`. When you build structures in the Workspace during the exercises that follow, you can save the structures in this project for later use.

# Building Small Molecules In Maestro

This chapter contains exercises on building new molecular structures from fragments and from individual atoms. You will use the structures you build in these exercises in the next chapter, to run various Jaguar calculations. For more detailed information about the Maestro Build panel tools, see Chapter 4 of the *Maestro User Manual*.

Before starting, you should ensure that the Default representation in the Settings tab of the Molecular Representation panel is Wire. You can open this panel from the Display menu.

## 2.1 Building a Structure by Placing Fragments

This exercise demonstrates how to build a structure from fragments, using Place mode. In this mode you can place molecular fragments in the Workspace, and substitute fragments in a structure in the Workspace.

1. If the Build toolbar is *not* displayed at the top of the Workspace, click the Show/Hide the build toolbar button.

   

   The Build toolbar is now displayed at the top of the Workspace.

2. Select the carbonyl fragment.

   
   

   The fragments are shown as full molecules, with H atoms added to the fragment to complete the molecule. The H atoms are replaced when you join fragments. The carbonyl fragment therefore appears as a formaldehyde molecule. If you pause the pointer over the fragment, the fragment name is displayed in the tooltip (Balloon Help).

3. Click in the Workspace.

   A formaldehyde molecule is placed in the Workspace.

4. Select the methyl fragment.

   
   

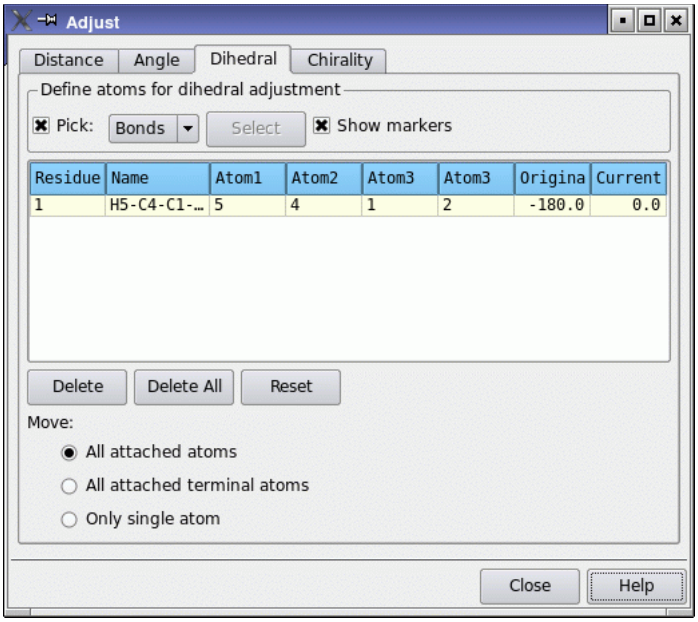


***Figure 2.1. The Dihedral tab in the Adjust panel.***

5. Click on one of the hydrogen atoms of the formaldehyde molecule in the Workspace.

   The hydrogen atom is replaced with a methyl fragment.

## 2.2 Adjusting a Dihedral Angle

In this exercise, you will change the orientation of the oxygen atom relative to the hydrogen atoms, so that there is a hydrogen atom cis to the oxygen atom.

1. Choose Edit > Adjust > Dihedral.

   The Adjust panel is displayed with the Dihedral tab on top.

2. Choose Bonds from the Pick menu.

3. Click on the C–C bond towards the carbonyl end.

   The H–C–C–O dihedral with the H trans to the O should be selected; the dihedral angle should be 180° (to within a sign). The selected atoms appear in the table in the center of the Dihedral tab. A broken line and an arrow mark the selected dihedral in the Workspace.

4. Change the value in the Current column to `0` and press ENTER.

   The dihedral is not adjusted if you do not press ENTER.

5. Click the Delete button to remove the defined dihedral from the list.

   The dihedral marker in the Workspace is removed.

6. Close the Adjust panel.

## 2.3 Saving Workspace Contents as a Project Entry

To model the interconversion between acetaldehyde and vinyl alcohol, you will need to convert the acetaldehyde structure to vinyl alcohol. Before proceeding, save the aldehyde molecule as a Project Table entry. This allows you to store the aldehyde structure while you construct the alcohol. The Project Table entries are also used to select reactant and product structures for transition state searches and IRC scans.

1. Click the Create entry from Workspace button on the main toolbar.

   

   The Create Entry From Workspace dialog box is displayed.

2. Type `aldehyde` in the Title text field and click Create.
3. Click the Open/Close project table button on the toolbar.

   

   The Project Table panel is displayed with the new entry as the first entry.

## 2.4 Duplicating Project Entries

In this exercise, you will copy the acetaldehyde entry you have generated to create a new entry for vinyl alcohol.

1. In the Project Table panel, ensure that the `aldehyde` entry is selected.
2. Type CTRL+D.

   A copy of the `aldehyde` entry is made. The new entry is automatically selected.

3. Click the title of the new entry to edit it.
4. Change the title to `alcohol` and press ENTER.
5. Change the entry name of the new entry to `alcohol` using the same procedure.

   If the entry name is not displayed, choose Property > Show Entry Name.

## 2.5 Converting the Acetaldehyde Structure Into Vinyl Alcohol

In this exercise, you will convert the copy of the acetaldehyde structure into vinyl alcohol by breaking the C–H bond, changing the bond orders, and then connecting the unattached hydrogen to the oxygen atom. Converting structures is especially useful for transition state searches when a reactant and a product structure is given, because the search relies on a consistent atom numbering scheme.

1. In the Project Table panel, click the In box of the `alcohol` entry.

   The `alcohol` entry is included in the Workspace and the `aldehyde` entry is excluded from the Workspace. Since the two entries are identical, there is no visible change in the Workspace.

2. Choose Bonds from the Delete button menu on the toolbar.

   

3. In the Workspace, click on the C–H bond cis to the C=O bond.

   The bond disappears and the H atom is represented by an asterisk.

4. Click the Decrement bond order button on the Build toolbar.

   

5. In the Workspace, click on the C=O bond.

   The bond should now be represented by a single line, indicating a single bond.

6. Click the Increment bond order button on the Build toolbar.

   

7. In the Workspace, click on the C–C bond.

   The bond should now be represented by a double line, indicating that the bond order has changed to double.

8. Click the Draw structures button on the Build toolbar.

   

9. In the Workspace, click on the oxygen atom, then click twice on the unbonded hydrogen.

   A bond is drawn between the two atoms.

## 2.6 Cleaning Up the Geometry

In this exercise, you will clean up the geometry by performing a force-field calculation that provides good estimates of the bond lengths and angles.

- Click the Clean up geometry Build toolbar button.

  

  A dialog box is displayed that shows cleanup progress.

You should always clean up structures before optimizing them. If the molecule has symmetry, always symmetrize the molecule before cleaning up the geometry, to guarantee perfect point group symmetry and to speed up the Jaguar calculation. In this exercise, the structure already has $C_s$ symmetry, so it is not necessary to symmetrize it. To symmetrize a molecule, choose Edit > Symmetrize Workspace in the main window.

The changes to this structure should be automatically saved in the project. If your project preferences (Project tab, Preferences panel) are not set to synchronize Workspace changes automatically, you should see a red exclamation point in the status bar of the main window. Click this icon to save the changes, and reset your preferences to automatic synchronization.

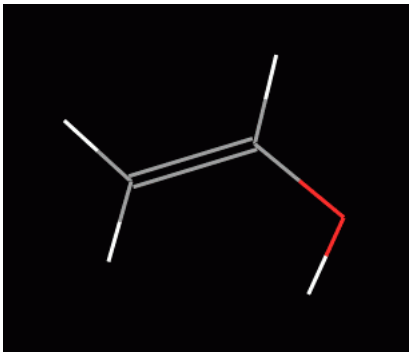

***Figure 2.2. The completed vinyl alcohol structure.***

## 2.7 Building a Structure by Growing Fragments

In this exercise, you will use fragments to build a structure as you did in the previous exercise. However, this time you will build in Grow mode. In this mode, selected fragments are combined using predefined *grow bonds*. The grow bond is the bond that is replaced when another fragment is selected in Grow mode. The fragment is added in an orientation that is determined by the choices made from the Grow direction and Joining geometry option menus.

1. Click the Clear Workspace button on the toolbar.

2. From the Show/hide the build toolbar button menu on the toolbar, choose Fragments.

The Build panel is displayed, with the Fragments tab on top and the organic fragments library displayed (see Figure 2.3).

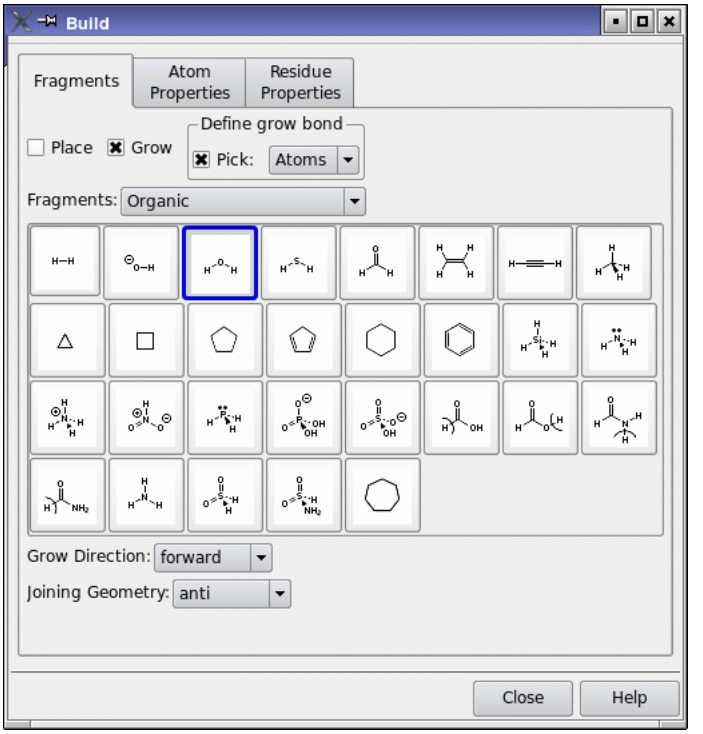


***Figure 2.3. The Build panel, showing the Fragments tab.***

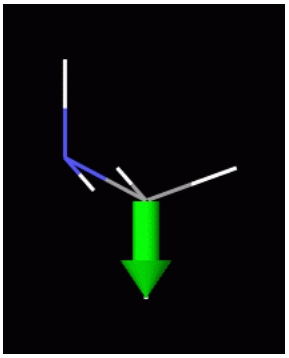

*Figure 2.4. The methylamine molecule showing the grow bond.*

3. Select Grow.
4. In the Organic library, click the Amine fragment.

   An amine group is placed in the Workspace. The green arrow marks the grow bond.
5. Click the Methyl fragment.

   A methyl group is attached to the amine group.
6. Create a Project Table entry named `methylamine`.

   See Section 2.3 on page 7 if you unsure of how to do this.

## 2.8 Building a Structure by Drawing

In this exercise, you will draw a benzene molecule in the Workspace. Although drawing benzene is not necessary because there is a benzene fragment in the organic fragment library, drawing structures can be useful when it is difficult to build them from fragments, such as structures with multiple fused rings.

1. Clear the Workspace.
2. Click the Draw structures button on the Build toolbar.

   

   The button is indented to indicate that Draw mode is active.The default atom selected for drawing is carbon. If you want to choose a different atom, click and hold on the button and select an element from the menu that is displayed.

3. Click once in the Workspace.

   An asterisk appears enclosed in a purple cube. This cube marks the active drawing atom. When there is an active drawing atom, clicking again in the Workspace while in Draw mode places another atom and bonds it to the original atom. Clicking a second time on the active drawing atom makes it inactive.

4. Draw a six-membered ring by clicking in the Workspace five more times in the proper configuration, then clicking on the first atom.

   As you move the mouse, a yellow line connects the pointer to the active atom. The atoms are all placed in the same plane.

5. Click the first atom a second time to end the draw operation.

## 2.9 Adjusting Bond Orders and Adding Hydrogens

In this exercise, you will adjust the C–C bond orders and add hydrogen atoms to the skeleton structure that you drew. You could also create the double bonds and add the hydrogens using Draw mode.

1. Click the Increment bond order button on the Build toolbar.

   

   The "B" below the cursor box indicates that the current selection state is Bonds.

2. Click a bond in the structure you just drew.

   The line representing the bond on which you clicked should now appear as a double line.

3. Click two more bonds to create a structure with alternating double bonds.

4. Double-click the Add hydrogens button.

   

   The double-click applies the selected hydrogen treatment to all atoms. The default treatment is All-atom with No-Lp. You can select the treatment in the Hydrogen Treatment panel, which you open from the Edit menu.

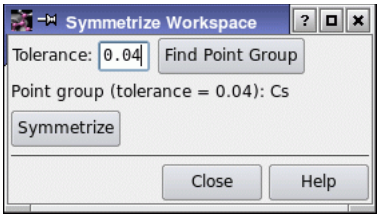


*Figure 2.5. The Symmetrize Workspace dialog box.*

## 2.10 Symmetrizing a Structure

The molecule you drew is planar, but is likely to have no other symmetry. In this exercise you will symmetrize the structure so that it has full $D_{6h}$ symmetry, then clean up the structure.

1. From the Edit menu, choose Symmetrize Workspace.

   The Symmetrize Workspace panel is displayed. The symmetry is likely to be $C_s$. The Find Point Group button is dimmed, because the structure actually has the symmetry displayed.

2. If the point group is not $D_{6h}$, increase the tolerance and click Find Point Group until the correct symmetry is located.

3. Click Symmetrize.

   The structure takes on the correct symmetry.

4. Clean up the structure (use the Clean up geometry toolbar button).

5. Check in the Symmetrize Workspace panel that the point group symmetry is still $D_{6h}$. If not, click Symmetrize.

   This second symmetrization may be necessary because the geometry cleanup perturbs the structure away from its symmetry to ensure that a minimum is found.

6. Close the Symmetrize Workspace panel.

7. Create a Project Table entry named `benzene` (see Section 2.3 on page 7).

# Running Jaguar Calculations

This chapter is designed to introduce you to the main capabilities of Jaguar 7.6 and its interface with Maestro 9.0.

## 3.1 Single Point Calculation

The default single-point energy calculation set up in Maestro is a density-functional calculation with the B3LYP functional and a 6-31G** basis set. The molecule is assumed to be singlet and uncharged. To run a default calculation, you can build or include a molecule in the Workspace and submit the job with no special options. In this exercise, you will use the molecule that you built in Section 2.8 on page 11. If you have not done this exercise, do so now.

1. In the Project Table panel, click the In column for the `benzene` entry.

   The `benzene` entry is included in the Workspace and all others are excluded.

2. From the Applications menu, choose Jaguar > Single Point Energy.

   The Jaguar panel is displayed, set up for a single-point energy calculation. The default structure, as shown in the Use structures from option menu, is the one in the Workspace.

3. Click the Start button.

   The Jaguar - Start dialog box opens. This dialog box provides controls for the running of the job and the incorporation of the results into Maestro. By default, the job name is the entry name and the job is run on the local host (the host on which you are running Maestro).

4. In the Output section, choose Incorporate > Append new entries individually.

   The incorporation mode is persistent, so the next time you run a job, the mode selected is the last mode that you used.

5. (*optional*) In the Job section, choose a host from the Host option menu.

6. Click Start.

   The Monitor panel is displayed, allowing you to monitor the progress of the job. This job should take only a few seconds.

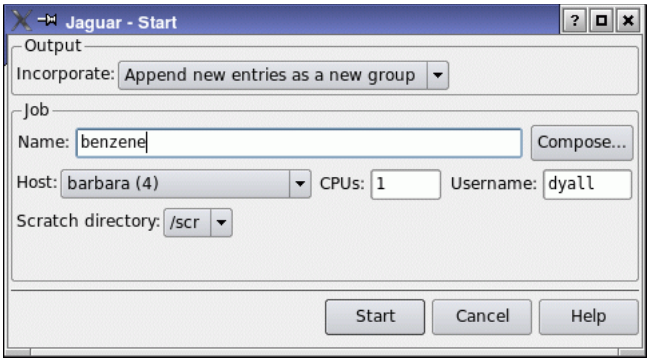


*Figure 3.1. The Jaguar - Start dialog box.*

7. When the job finishes, close the Monitor panel.

   The results of the job are incorporated into Maestro, and a new entry named `benzene` appears in the Project Table.

## 3.2 Geometry Optimization With DFT

In this exercise, you will optimize the geometry of the output structure from the previous exercise, at the BLYP/6-31G** level.

1. In the Jaguar panel, click Read (at the bottom of the panel).

   The Jaguar Read file chooser is displayed. If you do not have the Jaguar panel open, choose Applications > Jaguar > Single Point Energy in the main window.

2. Navigate to and select the Jaguar restart file, `benzene.01.in`.

   The restart file contains the geometry and wave function for the single point calculation performed in the last exercise.

3. Ensure that Read As is set to Geometry and settings.

4. Click Open.

   In the Project Table a new entry, `benzene.01`, has appeared and has been included automatically in the Workspace.

   You can view the input file information by clicking the Edit button in the Jaguar panel. Do not change any of the settings, but notice that in the **guess** section there is now a converged wave function. Close the panel by clicking Cancel.

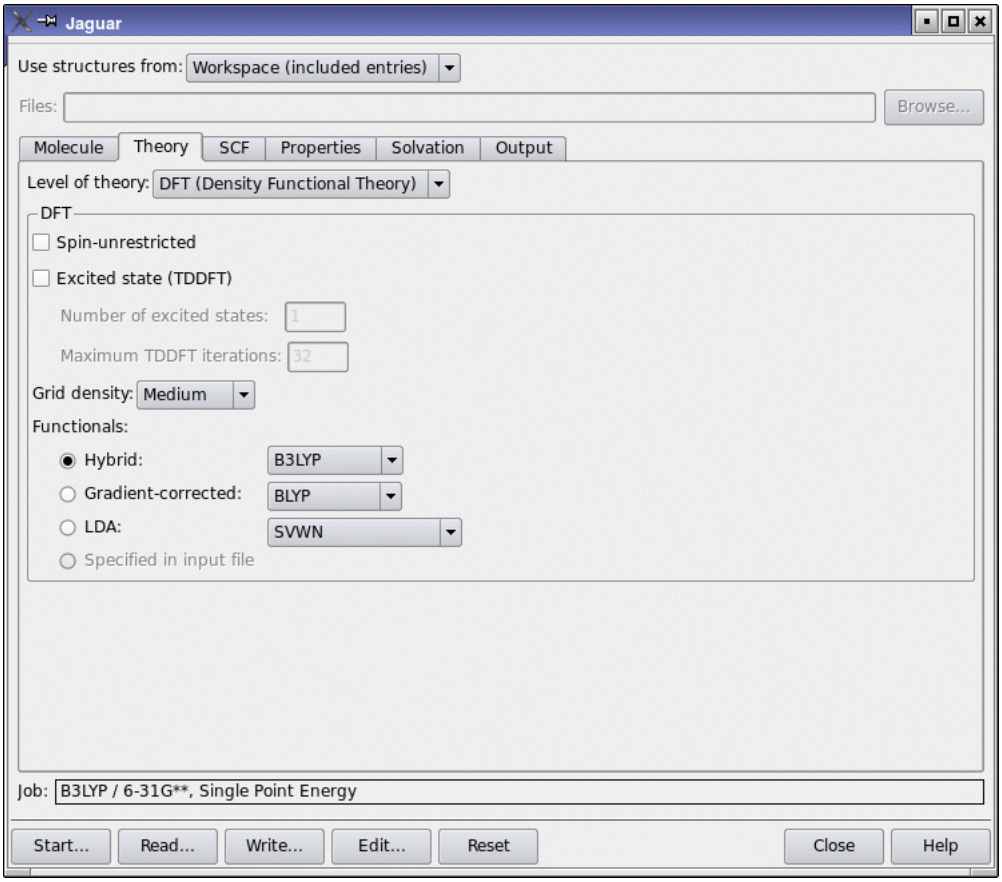


***Figure 3.2. The Theory tab of the Jaguar panel.***

5. Choose Applications > Jaguar > Optimization in the main window.

   The Jaguar panel is displayed, set up for a geometry optimization.

6. In the Theory tab, select Gradient-corrected in the Functionals section, then choose BLYP from the corresponding option menu.

   You can view the input file contents by clicking the Edit button. Notice the addition of keywords in the **gen** section. A BLYP calculation is specified by `dftname=blyp` and a geometry optimization is specified by `igeopt=1`. Close the panel by clicking Cancel.

7. Click Start.

   The Start dialog box opens.

8. (*optional*) In the Job section, choose a host from the Host option menu.

9. Type `benzene_dft` in the Name text box, and click Start.

The Monitor panel is displayed and shows the job's progress. This job takes a few minutes to finish. When it has finished, close the Monitor panel. A new entry named `benzene.01` appears in the project table.

## 3.3 Localized MP2 Energy Calculation

In this exercise, you will determine the MP2 energy of benzene at the DFT geometry.

1. Read the restart file `benzene_dft.01.in`, as Geometry and settings.

   This file contains the optimized geometry of benzene from the previous exercise. See page 16 for instructions about reading files. A new project entry is created.

2. Choose Applications > Jaguar > Single Point Energy in the main window.

3. In the Theory tab, choose LMP2 (local MP2) from the Level of theory option menu.

Since benzene is aromatic, you should use a special form of LMP2, which allows all the electron pairs of the ring to be excited into an expanded virtual space (a semi-delocalized LMP2). This can be achieved automatically by adding keywords directly to the input file.

4. Click Edit.

   The Edit Job panel is displayed.

5. In the `&gen` section, add `idelocv=1` and `ireson=1`.

6. Click OK.

7. In the Jaguar panel, click Start.

   The Start dialog box opens.

8. (*optional*) In the Job section, choose a host from the Host option menu.

9. Type `benzene_mp2` in the Name text box, and click Start.

   This LMP2 job takes several minutes. When the job has finished, close the Monitor panel.

10. Examine the output file, `benzene_mp2.out`, using a text editor.

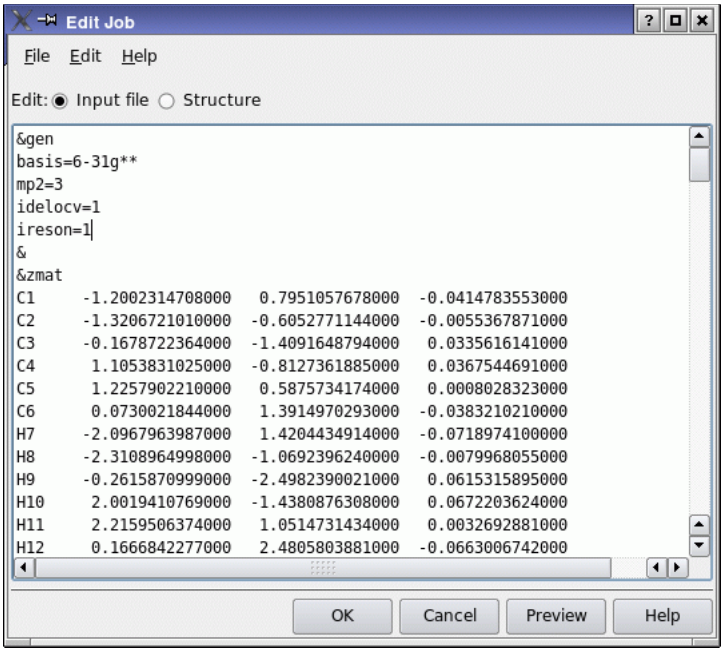


***Figure 3.3. The Edit Job panel showing the new gen section contents.***

## 3.4 Displaying Orbitals in Maestro

Maestro can display surfaces, including orbital and density plots generated by Jaguar. In this exercise, you will see how to produce and display orbital plots. You will use the output from the DFT calculation you ran earlier to generate and display a surface plot of the HOMO and LUMO of benzene.

The generation of surfaces require a wave function. For this exercise the wave function is obtained from the restart file, but surfaces can be generated at the end of any job. However, no SCF iterations are needed, so an initial guess calculation is sufficient to generate the surfaces.

1. Read the restart file, `benzene_dft.01.in`, as Geometry and settings.

   A new project entry is created and included in the Workspace.

2. From the menu, choose Jaguar > Initial Guess Only.

3. In the Theory tab, check that the level of theory is DFT.

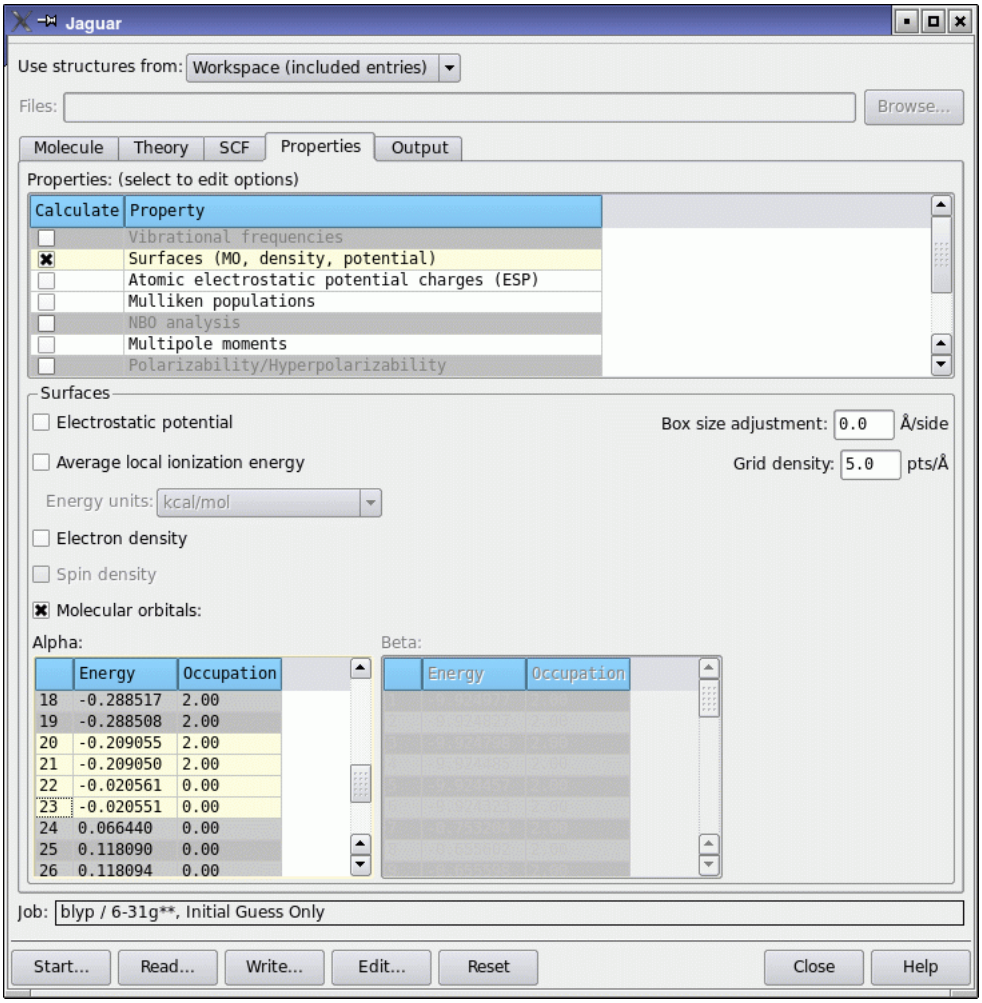


***Figure 3.4. The Properties tab.***

4. In the Properties tab, select the check box in the Surfaces row.

   Controls for the selection of surfaces are displayed in the lower part of the tab. If you have a wave function, these controls include a list of orbitals with their occupation number and eigenvalue. If you do not have a wave function, the controls allow you to specify the range of orbitals to plot relative to the HOMO and the LUMO.

5. Select Molecular Orbitals.

6. From the Alpha list, select orbitals 20 through 23 (click 20, shift-click 23).

7. Click Start.

   The Start dialog box opens.

8. (*optional*) In the Job section, choose a host from the Host option menu.

9. Type `benzene_mo` in the Name text box, choose Replace existing entries from the Incorporate option menu, then click Start.

10. When the job has finished, close the Monitor panel.

    The job takes about one minute. The results are automatically incorporated and the first surface (the HOMO) is displayed in the Workspace. Since both the HOMO and the LUMO are degenerate orbitals, the orbital displayed could be either of the degenerate pair.

11. If the Project Table panel is not open, click the Open/Close project table button on the toolbar.

12. In the Project Table, click the S button in the Aux column for the benzene entry.

    The Manage Surfaces panel is displayed. The Surface Table shows all the surfaces generated by the Jaguar job.

13. Click the V column for orbital 21.

    Orbital 21 replaces orbital 20 in the Workspace.

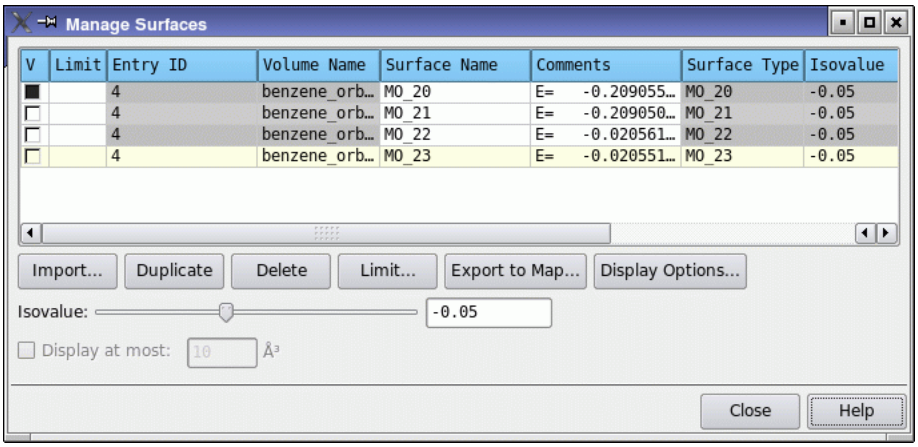


***Figure 3.5. The Manage Surfaces panel.***

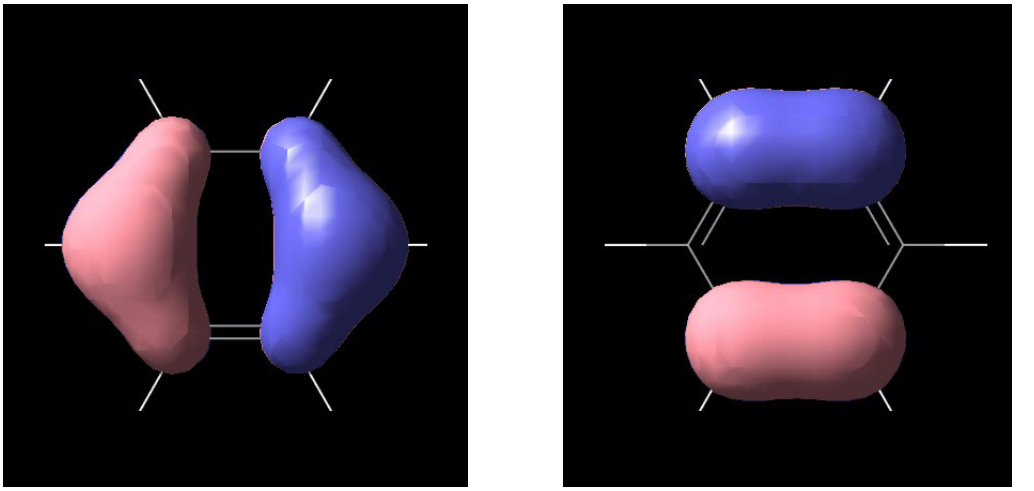

*Figure 3.6. The degenerate benzene HOMO molecular orbitals*

14. Move the Isovalue slider.

    The volume occupied by the orbital changes with the isovalue.

15. Reset the isovalue to –0.05.

16. Click Display Options.

    The Display Options dialog box is displayed. This dialog box has controls for the style, transparency, and color scheme.

17. Experiment with changing the transparency, the style, and the colors of the positive and negative lobes.

    For this manual, the colors of the surfaces were changed for better grayscale printing.

18. Display the remaining two orbitals.

To save images of the Workspace like those shown in Figure 3.6, choose Maestro > Save Image, then make settings and supply a filename in the Save Image panel.

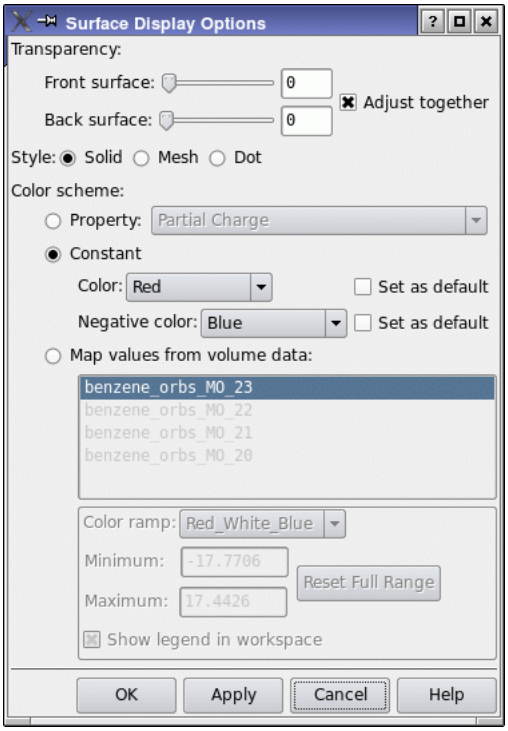


***Figure 3.7. The Display Options dialog box.***

## 3.5 Transition State Search

In this exercise, you will model the interconversion between acetaldehyde and vinyl alcohol, which involves the transfer of a proton from the methyl group to the carbonyl oxygen. You will use the vinyl alcohol and acetaldehyde molecules that you built in Chapter 2 as the starting and ending structures. If you have not yet built these structures, build them now.

1. In the Project Table panel, shift-click to select the alcohol and aldehyde entries, and click the In box of the `alcohol` entry.
2. Choose Applications > Jaguar > Transition State Search in the main window.
3. Click Reset.
4. In the Molecule tab, check that the basis set is 6-31G**.
5. Choose Off from the Symmetry option menu.
6. In the Theory tab, make selections for a BLYP DFT calculation.

   BLYP is in the Gradient-corrected option menu.

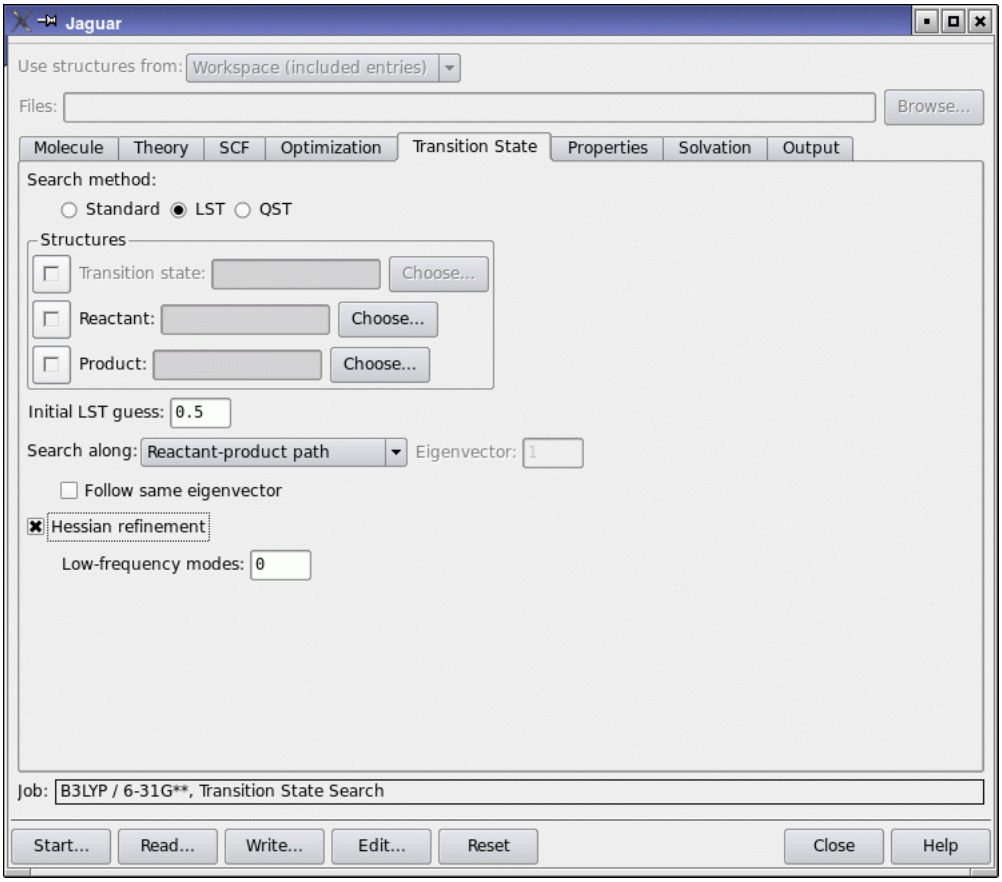


***Figure 3.8. The Transition State tab.***

7. In the Transition state tab (see Figure 3.8), under Search method, select LST.

   The Reactant and Product rows in the Structures section are now available.

8. In the Reactant row, click Choose.

   The Choose Entry dialog box is displayed.

9. Select alcohol from the list, then click Choose.

   The dialog box closes, and the Reactant text box now contains `alcohol`. The `alcohol` entry has been selected as the reactant.

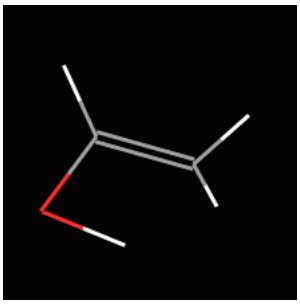

*Figure 3.9. The transition state structure.*

10. In the Product row, click Choose.

    The Choose Entry dialog box is displayed again.

11. Select aldehyde from the list, then click Choose.

    The dialog box closes, and the Product text box now contains `aldehyde`. The `aldehyde` entry has been selected as the product.

12. In both rows, click the box to the left of the text box.

    The aldehyde structure is displayed in the Workspace on top of the alcohol structure.

13. Click Start.

    The Start dialog box opens.

14. (*optional*) In the Job section, choose a host from the Host option menu.

15. Set the name to `trans_state`, choose Append new entries individually from the Incorporate option menu, and click Start.

    Convergence should be reached in about 13-15 geometry steps. When the job finishes, the results are incorporated into the Project Table as a new entry. The structure shows the H atom bonded to the O atom with an elongated bond.

## 3.6 Vibrational Frequencies

In this exercise, you will calculate the vibrational frequencies of the transition state you found in the previous exercise and view an animation of the frequencies in Maestro.

1. Ensure that the transition state entry is the only selected entry in the Project Table.
2. Choose Applications > Jaguar > Single Point Energy in the main window.
3. Choose Selected entries from the Use structures from option menu.

4. In the Properties tab, select the check box for Vibrational frequencies.
5. Click Start.

   The Start dialog box opens.
6. (*optional*) In the Job section, choose a host from the Host option menu.
7. Set the name to `trans_freq` and click Start.

   This job takes several minutes to finish, and generates a `.vib` file that Maestro uses for animation of frequencies. When the results are incorporated, a V is added to the Aux column in the Project Table for the incorporated entry.
8. Click the V button in the Aux column of the project table for the incorporated entry.

   The Vibration panel is displayed.
9. Select the first frequency in the list, then select Animate.

   This is the imaginary frequency that corresponds to the transition state. The frequency is animated in the Workspace as if it were real. The structure can be rotated in the Workspace to view the animation from an optimal angle.
10. Click on other frequencies in the list to animate them. Experiment with adjusting the speed and amplitude.

    You do not need to deselect Animate to change to a different frequency.

The file `trans_freq.out` contains a list of frequencies and normal modes below the heading `start of program freq`. Below the frequencies is information on the zero point energy, entropy, and other thermodynamic quantities.

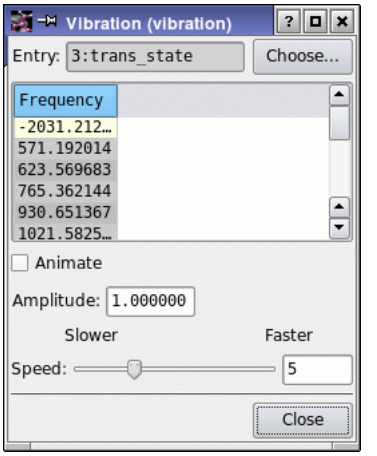


***Figure 3.10. The Vibration panel.***

## 3.7 Intrinsic Reaction Coordinate Calculation

In this exercise you will use the results of the transition state search and frequency calculation from the previous exercises to perform an intrinsic reaction coordinate scan, and visualize the reaction in Maestro with the ePlayer.

1. In the Jaguar panel, click Read.

   The Jaguar Read dialog box is displayed.

2. Select Geometry and settings from the Read As option menu.

3. Read the restart file `trans_freq.01.in` from the previous exercise.

   The transition state structure is displayed in the Workspace and incorporated into the Project Table. The hydrogen atom is located, as expected, about halfway between its starting and ending position.

   To perform an IRC scan, you must read or generate a Hessian. In this case the Hessian is read from the restart file, `trans_freq.01.in`.

4. In the Project Table, click to select the transition state structure.

5. Choose Applications > Jaguar > Reaction Coordinate in the main window.

   You must choose the task after reading the input file because reading an input file with its settings sets the Jaguar task to the task defined by the **gen** section of the input file.

6. In the Properties tab, clear the Vibrational frequencies check box.

7. In the IRC tab, click Choose in the Transition state row of the Structures section.

   The Choose Entry dialog box is displayed.

8. Select the structure you just read in.

9. Click Choose in the Reactant row of the Structures section, and select the original alcohol entry.

   If the alcohol structure is not listed in the Choose Entry panel, then select All from the Choose entry from menu.

10. Click Choose in the Product row, and select the original aldehyde entry.

11. Click Start.

    The Start dialog box opens.

12. (*optional*) In the Job section, choose a host from the Host option menu.

13. Set the name to `irc`, choose Append new entries as a new group from the Incorporate option menu, and click Start.

The job takes a few minutes. When the job finishes, 13 new entries are incorporated into the Project Table as an entry group named `irc`, and are selected. The first entry corresponds to the transition state structure, the next six are the geometries found moving in the forward direction, from the transition state to the alcohol, and the last six are from the backward direction, moving toward the aldehyde structure. To view the reaction in the ePlayer, the entries must first be sorted. It is also useful to display the structures in Ball & Stick representation.

1. In the Project Table, include all 13 output structures in the Workspace. (To do this, click the In column for the first entry and shift-click the last entry.)
2. Double-click the Draw atoms in ball and stick button on the main toolbar.

3. Clear the Workspace.
4. In the Project Table, click the Sort button on the toolbar.

The Sort Project Table panel is displayed.

5. Select Rxn coord as the Primary Key and change the Order to Descending.

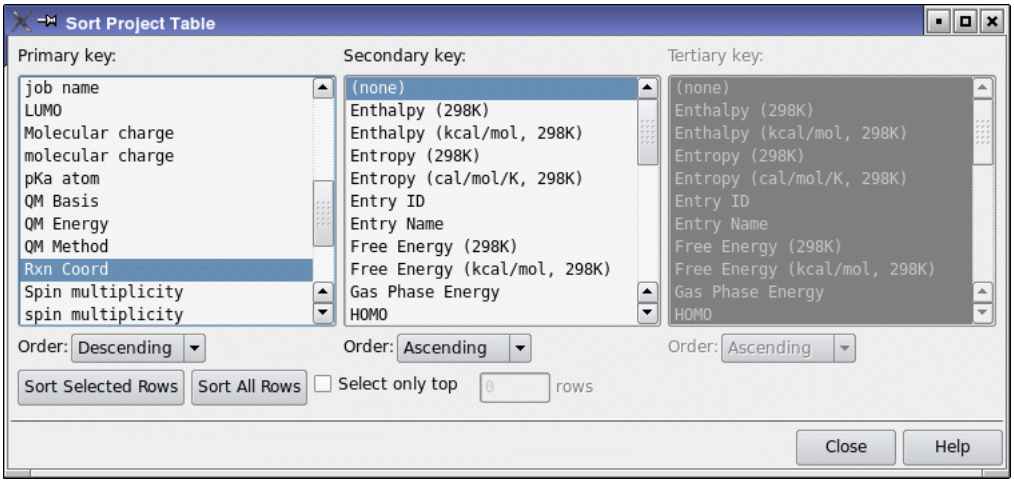


***Figure 3.11. The Sort Project Table panel.***

6. Click Sort Selected Rows, then click Close.
7. Click the Play forward button on the toolbar to start cycling through the entries.

   

   The hydrogen atom moves away from the oxygen and the double bond rotates.
8. From the Loop button menu on the toolbar, choose Oscillate.

   
9. Click the Play forward button.
10. The sequence of structures is played in the forward direction, then the reverse direction, and continues this pattern.
11. Click the Stop button.

    

You can change the speed of the ePlayer and set other options in the ePlayer Options panel, which you open from the ePlayer menu.

## 3.8 Prediction of p$K_a$ Values

In this exercise, you will calculate the p$K_a$ of methylamine, using the structure you built in an earlier exercise.

1. Include the methylamine molecule in the Workspace.
2. From the Applications menu, choose Jaguar > pKa.

   The Jaguar panel opens with the Molecule tab displayed. The controls in this tab are simplified. In the lower section, you can specify the p$K_a$ atom. Use this atom is selected by default.
3. In the pKa atom section, select Pick.
4. Click on the nitrogen atom in the Workspace.

   The nitrogen atom is marked and its label is displayed in the text box.
5. Select Workspace from the Use structures from option menu.

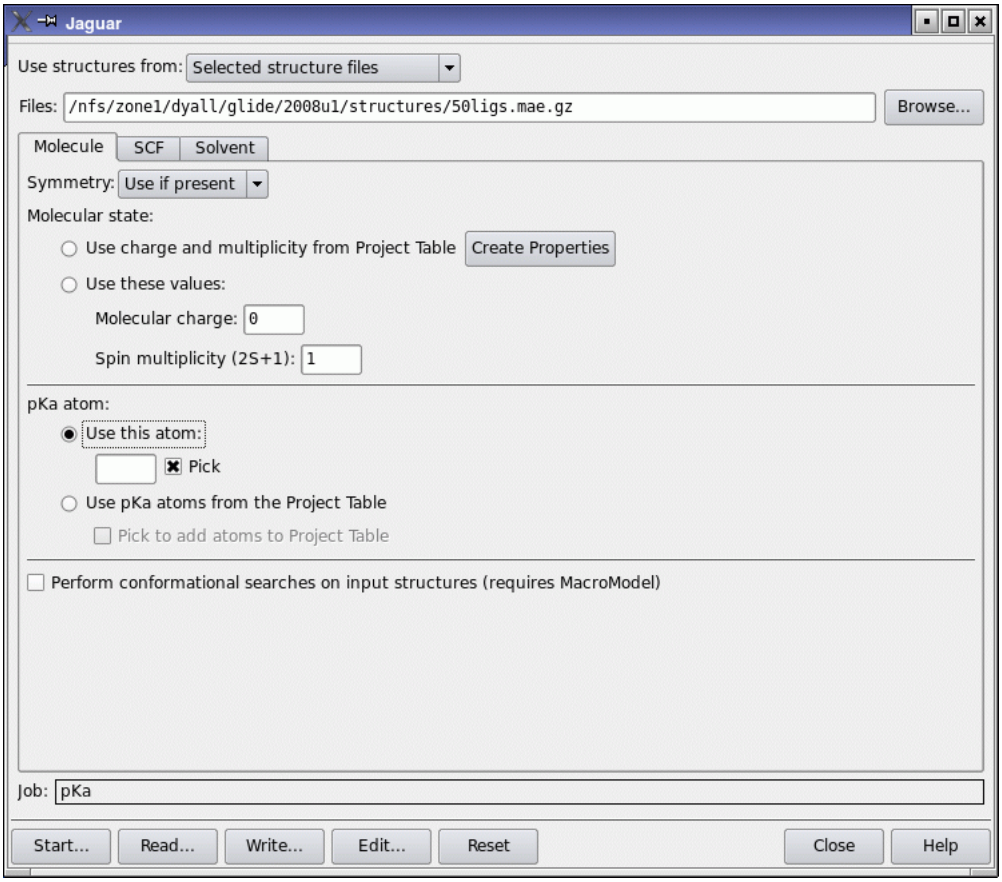


***Figure 3.12. The Molecule tab for p$K_a$ calculations.***

6. Click Start.

   The Start dialog box opens.

7. (*optional*) In the Job section, choose a host from the Host option menu.

8. Choose Replace existing entries from the Incorporate option menu.

9. Set the job name to `pka` and click Start.

The calculation of p$K_a$ values involves a number of steps and can be time-consuming. This job takes several minutes to finish. The output p$K_a$ is the only data written to the file `methylamine.out`. When the job finishes, the p$K_a$ value is added to the methylamine entry as a property.

# Getting Help

Schrödinger software is distributed with documentation in PDF format. If the documentation is not installed in `$SCHRODINGER/docs` on a computer that you have access to, you should install it or ask your system administrator to install it.

For help installing and setting up licenses for Schrödinger software and installing documentation, see the *Installation Guide*. For information on running jobs, see the *Job Control Guide*.

Maestro has automatic, context-sensitive help (Auto-Help and Balloon Help, or tooltips), and an online help system. To get help, follow the steps below.

- Check the Auto-Help text box, which is located at the foot of the main window. If help is available for the task you are performing, it is automatically displayed there. Auto-Help contains a single line of information. For more detailed information, use the online help.
- If you want information about a GUI element, such as a button or option, there may be Balloon Help for the item. Pause the cursor over the element. If the Balloon Help does not appear, check that Show Balloon Help is selected in the Maestro menu of the main window. If there is Balloon Help for the element, it appears within a few seconds.
- For information about a panel or the tab that is displayed in a panel, click the Help button in the panel, or press F1. The help topic is displayed in your browser.
- For other information in the online help, open the default help topic by choosing Online Help from the Help menu on the main menu bar or by pressing CTRL+H. This topic is displayed in your browser. You can navigate to topics in the navigation bar.

The Help menu also provides access to the manuals (including a full text search), the FAQ pages, the New Features pages, and several other topics.

If you do not find the information you need in the Maestro help system, check the following sources:

- *Maestro User Manual*, for detailed information on using Maestro
- *Maestro Command Reference Manual*, for information on Maestro commands
- *Maestro Overview*, for an overview of the main features of Maestro
- *Maestro Tutorial*, for a tutorial introduction to basic Maestro features
- *Jaguar User Manual*, for detailed information on using Jaguar
- Jaguar Frequently Asked Questions pages, at https://www.schrodinger.com/Jaguar_FAQ.html

- Known Issues pages, available on the Support Center.

The manuals are also available in PDF format from the Schrödinger Support Center. Local copies of the FAQs and Known Issues pages can be viewed by opening the file `Suite_2009_Index.html`, which is in the `docs` directory of the software installation, and following the links to the relevant index pages.

Information on available scripts can be found on the Script Center. Information on available software updates can be obtained by choosing Check for Updates from the Maestro menu.

If you have questions that are not answered from any of the above sources, contact Schrödinger using the information below.


E-mail: help@schrodinger.com
USPS: Schrödinger, 101 SW Main Street, Suite 1300, Portland, OR 97204
Phone: (503) 299-1150
Fax: (503) 299-4532
WWW: http://www.schrodinger.com
FTP: ftp://ftp.schrodinger.com


Generally, e-mail correspondence is best because you can send machine output, if necessary. When sending e-mail messages, please include the following information:

- All relevant user input and machine output
- Jaguar purchaser (company, research institution, or individual)
- Primary Jaguar user
- Computer platform type
- Operating system with version number
- Jaguar version number
- Maestro version number
- mmshare version number

On UNIX you can obtain the machine and system information listed above by entering the following command at a shell prompt:

```
$SCHRODINGER/utilities/postmortem
```

This command generates a file named *username*`-`*host*`-schrodinger.tar.gz`, which you should send to help@schrodinger.com. If you have a job that failed, enter the following command:

```
$SCHRODINGER/utilities/postmortem jobid
```

where *jobid* is the job ID of the failed job, which you can find in the Monitor panel. This command archives job information as well as the machine and system information, and

includes input and output files (but not structure files). If you have sensitive data in the job launch directory, you should move those files to another location first. The archive is named *jobid*`-archive.tar.gz`, and should be sent to help@schrodinger.com instead.

If Maestro fails, an error report that contains the relevant information is written to the current working directory. The report is named `maestro_error.txt`, and should be sent to help@schrodinger.com. A message giving the location of this file is written to the terminal window.

More information on the `postmortem` command can be found in Appendix A of the *Job Control Guide*.

On Windows, machine and system information is stored on your desktop in the file `schrodinger_machid.txt`. If you have installed software versions for more than one release, there will be multiple copies of this file, named `schrodinger_machid-`*N*`.txt`, where *N* is a number. In this case you should check that you send the correct version of the file (which will usually be the latest version).

If Maestro fails to start, send email to help@schrodinger.com describing the circumstances, and attach the file `maestro_error.txt`. If Maestro fails after startup, attach this file and the file `maestro.EXE.dmp`. These files can be found in the following directory:

```
%LOCALAPPDATA%\Schrodinger\appcrash
```

On Windows XP and Windows 2000, `%LOCALAPPDATA%` is not set by default, but should correspond to `%USERPROFILE%\Local Settings\Application Data`.

120 West 45th Street, 17th Floor
New York, NY 10036

101 SW Main Street, Suite 1300
Portland, OR 97204

8910 University Center Lane, Suite 270
San Diego, CA 92122

Zeppelinstraße 13
81669 München, Germany

Dynamostraße 13
68165 Mannheim, Germany

Quatro House, Frimley Road
Camberley GU16 7ER, United Kingdom

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